SAND2000-8527C

Combined pdf-sdf approach to partially premixed turbulent combustion

WOLFGANG KOLLMANN
MAE Department
University of California
Davis, CA 95616
and
JACQUELINE H. CHEN and HONG G. IM
Combustion Research Facility, Mail Stop 9051
Sandia National Laboratories
Livermore, California 94551-0969

Corresponding author:
Wolfgang Kollmann
MAE Department
University of California
Davis, CA 95616, USA
Phone: (530) 752-1452
Fax: (530) 752-4158
email: wkollmann@ucdavis.edu

Word Count:
text: 2310 (text) + 567 (equations) + 241 (references)
figures: 1200 (6 × 200)
total: 4318

Preferred Presentation:
Poster

Preferred colloquium topic area:
Turbulent flames (premixed)

Submitted to the 28th Symposium (International) on Combustion, Edinburgh, Scotland

Abstract

Partially premixed turbulent flames can develop flow regimes where triple flames emerge consisting of essentially premixed and non-premixed zones. The description of such phenomena requires a criterion for the detection of such zones. Such a criterion can be based on a wide range of variables including reaction rates, mass fractions of radicals, etc. These variables are not necessarily suitable for the limit of infinitely fast reactions, for instance, reaction rates are obviously not bounded in this limit. Hence a new single scalar variable based on geometric properties of mixture fraction and non-conserved variables is constructed, that allows the detection of finite rate and, in particular, triple flame domains and is bounded in the limit of infinitely fast reactions. This is first done for systems with simplified chemistry described by two variables and then generalized to combustion with complex chemistry. A pdf-sdf formalism is then outlined for the local thermodynamic state conditioned upon the degree of finite rate effects.

Finite rate and triple flame zones

Finite rate chemistry and transport effects in partially premixed flames are responsible for the appearance of triple flames ([10], [14], [15], [13]). The DNS results of Echekki and Chen[13] provide the detailed account of the structure of triple flames suitable for the development of a combined pdf/sdf formalism for turbulent flames.

Suppose the local thermodynamic properties can be determined by two scalar variables: Mixture fraction $Z(\mathrm{x}, t)$ and a progress variable $c(\mathrm{x}, t)$. The simplified chemical framework for the combustion of methane with air proposed by Linan and Williams [12] verifies that this is possible. Let the progress variable be proportional to temperature for the sake of argument. Consider now the results of Echekki and Chen[13] for the partially premixed Methanol-air flame. Their figure 8 shows the isolines for mixture fraction and temperature in the neighbourhood of the triple flame. It is clear from the geometry of these isolines that in the nonpremixed branches of the triple flame the isolines of mixture fraction and temperature align themselves, hence approach a local dependence of temperature on mixture fraction as can be expected for pure nonpremixed flames. On the other hand are the isolines for mixture fraction nearly orthogonal to the isolines of temperature near the head of the triple flame. These results indicate that a criterion for the detection of zones with finite rate effects and triple flames can be based on geometric properties of level surfaces in three dimensional and on level lines in two dimensional flows.

Assumptions

The criterion to be developed rests on a set of restrictions which can be stated as follows:

(1) The Navier-Stokes equations for the zero Mach number limit (Majda and Sethian [16]) hold.

(2) The conditions stated by Williams ([17], section 1.3) for the existence of coupling functions hold.

(3) The flow domain is open.

It follows from these conditions that the limit of infinitely fast chemistry reduces the system of thermodynamic variables governed by pdes to a single one called mixture fraction Z: Density, temperature and composition become local (not involving differential or integral expressions) functions of Z. Here the assumptions of zero Mach number and open domain are crucial since compressibility effects would make density and temperature nonlocal (i.e. via differential equations) functions of the velocity, energy and pressure fields and the zeroth order pressure would be time dependent in closed domains. It is possible to derive a compressible flame sheet model for infinitely fast reactions, but pressure, temperature and composition emerge as local functions of three variables: Mixture fraction, density and internal energy.

Geometric criterion: Two variables

Simplified chemistry involving only two variables (mixture fraction and a progress variable, all variables are assumed dimensionless) is considered first. The angle γ between the gradients of mixture fraction Z and progress variable c

$$\gamma = \sin^{-1}(|\mathrm{n}^Z \times \mathrm{n}^c|) \tag{1}$$

is according to the simulation results of Echekki and Chen [13] close to zero for regions without significant finite rate effects and large in the flame zones. The unit normal vectors for the level surfaces of mixture fraction and progress variables are defined by

$$\mathrm{n}^Z \equiv \frac{\nabla Z}{|\nabla Z|}, \quad \mathrm{n}^c \equiv \frac{\nabla c}{|\nabla c|} \tag{2}$$

The finite rate domain can be defined by $\mathcal{T} = \{\mathrm{x} : |\gamma| > \gamma_0\}$ where $\gamma_0 > 0$ is a suitable limit value. The progress variable c varies significantly near the flame zone, but can be expected to be close to zero or unity away from it. Hence, the computation of unit normal vectors may suffer from numerical inaccuracy away from the flame zones. This problem can be overcome by using

$$\mathrm{g} \equiv \frac{\nabla Z}{1 + |\nabla Z|} \times \frac{\nabla c}{\max|c| + |\nabla c|} \tag{3}$$

for the construction of a scalar detection function $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$. The vector g is proportional to the sinus of the angle between the two gradients, if $|\nabla Z| \gg 1$ and $|\nabla c| \gg \max|c|$ hold and it approaches the zero vector as one of the gradients vanishes. Hence, (3) is adopted in the following and the criterion for the detection of finite rate zones is stated as

$$\mathcal{F} > f_0 \tag{4}$$

where $\max \mathcal{F} \gg f_0 > 0$ is a suitable value. It fits the bill since $\mathcal{F}$ is close to zero if the gradients are close to parallel (approach of nonpremixed reaction zones) or if one of the gradients approaches zero (zones without reactions). Furthermore, this definition enjoys the advantage (in contrast to reaction rates) to be bounded as the limit of infinitely fast reactions is approached.

Generalisation to complex chemistry

This criterion can be generalized to partially premixed flames with complex chemistry where the local thermodynamic state is described by non-conserved variables c_i, $i = 1, \cdots, M$ and a mixture fraction variable Z. In the limit of infinitely fast reactions, all c_i become local functions of Z according to the assumptions stated above. The obvious generalisation would be to construct the scalar $\mathcal{F}$ as function of all the gradients of the M progress variables, which would align themselves with the gradient of mixture fraction, in the form

$$\mathcal{F} \equiv \sum_{i=1}^{M} \mathbf{g}_i \cdot \mathbf{g}_i \tag{5}$$

This would lead to extreme complexity of the transport pde for $\mathcal{F}$ and defeat the purpose to produce a tool for the analysis of finite rate regions in turbulent flames. However, the results presented below indicate that there is another possibility. Scalar variables such as temperature and density depend on all reaction steps in an implicit manner: The Navier-Stokes system for combustion flows in zero Mach number limit (see Majda and Sethian [16]) can be set up for the variables velocity, pressure, composition variables and internal energy, all satisfying pdes. Density and temperature follow then from local state relations, hence $\rho(v_\alpha, p, Y_1, \cdots, Y_N, u)$ and $T(v_\alpha, p, Y_1, \cdots, Y_N, u)$ with nonlocal (functional) dependence on velocity. The composition variables in turn are functions of the chemical rate parameters (Damkoehler numbers for the individual reactions), hence are density and temperature functions of these parameters. It follows that it is sufficient for complex systems of combustion reactions to consider the definition

$$\mathbf{g} \equiv \frac{\nabla Z}{1 + |\nabla Z|} \times \frac{\nabla \rho}{\max|\rho| + |\nabla \rho|} \tag{6}$$

(the dimensionless density is not necessarily positive) and

$$\mathcal{F} = \mathbf{g} \cdot \mathbf{g} \tag{7}$$

This definition satisfies the requirements for the detection of finite rate regions and remains bounded as infinitely fast reactions are approached.

Level surfaces enclosing triple flames

The construction of a scalar variable $\mathcal{F}$ (7) as the vector product of two gradients (6) allows the detection of regions in space with finite rate chemistry, which is the necessary condition for the appearance of triple flames. The scalar $\mathcal{F}$ is now used to outline a sdf/pdf formalism for the study of the processes responsible for the creation and destruction of such regions. In particular, the area of surfaces bounding finite rate regions and triple flames and their topological and geometric properties are of interest (Kollmann and Chen [1]).

Pde for the scalar defining the level surfaces

The pde for $\mathcal{F}$ (in Cartesian coordinates for simplicity) is determined by the pdes for mixture fraction Z

$$\rho\frac{DZ}{Dt} = \frac{1}{ReSc}\frac{\partial}{\partial x_\alpha}(\rho\mathcal{D}\frac{\partial Z}{\partial x_\alpha}) \tag{8}$$

and mass balance

$$\frac{D\rho}{Dt} = -\rho\nabla\cdot\mathrm{v} \tag{9}$$

where D/Dt is the substantial derivative, Re and Sc denote Reynolds and Schmidt numbers, $\mathcal{D}$ is the dimensionless mass diffusivity which depends on temperature and composition. The gradients are governed by

$$\frac{D}{Dt}(\frac{\partial Z}{\partial x_\alpha}) = \frac{1}{ReSc}\left\{\frac{\partial}{\partial x_\beta}(\mathcal{D}\frac{\partial^2 Z}{\partial x_\beta\partial x_\alpha}) + \frac{\partial}{\partial x_\alpha}(\frac{1}{\rho}\frac{\partial\rho}{\partial x_\beta})\mathcal{D}\frac{\partial Z}{\partial x_\beta} + \frac{1}{\rho}\frac{\partial\rho}{\partial x_\beta}\mathcal{D}\frac{\partial^2 Z}{\partial x_\beta\partial x_\alpha}\right\} - \frac{\partial v_\beta}{\partial x_\alpha}\frac{\partial Z}{\partial x_\beta} \tag{10}$$

and

$$\frac{D}{Dt}(\frac{\partial\rho}{\partial x_\alpha}) = -(\nabla\cdot\mathrm{v}\delta_{\alpha\beta} + \frac{\partial v_\beta}{\partial x_\alpha})\frac{\partial\rho}{\partial x_\beta} - \rho\frac{\partial}{\partial x_\alpha}(\nabla\cdot\mathrm{v}) \tag{11}$$

The pde for $\mathcal{F}$ is then determined by

$$\frac{\partial\mathcal{F}}{\partial t} = \frac{2\epsilon_{\alpha\beta\gamma}g_\alpha}{(1+|\nabla Z|)(\max|\rho|+|\nabla\rho|)}\left\{(\delta_{\beta\omega} - \frac{|\nabla Z|}{1+|\nabla Z|}n_\beta^Z n_\omega^Z)\frac{\partial}{\partial t}(\frac{\partial Z}{\partial x_\omega})\frac{\partial\rho}{\partial x_\gamma}\right.$$
$$\left. + (\delta_{\gamma\omega} - \frac{|\nabla\rho|}{\max|\rho|+|\nabla\rho|}n_\gamma^\rho n_\omega^\rho)\frac{\partial Z}{\partial x_\beta}\frac{\partial}{\partial t}(\frac{\partial\rho}{\partial x_\omega})\right\} \tag{12}$$

The resulting evolution equation for $\mathcal{F}$ is written in abbreviated form

$$\rho\frac{D\mathcal{F}}{Dt} = \frac{1}{ReSc}\frac{\partial}{\partial x_\alpha}(\rho\mathcal{D}\frac{\partial\mathcal{F}}{\partial x_\alpha}) + \rho Q \tag{13}$$

and

$$\Omega_\mathcal{F} = \frac{1}{ReSc}\frac{\partial}{\partial x_\alpha}(\mathcal{D}\frac{\partial\mathcal{F}}{\partial x_\alpha}) + Q \tag{14}$$

which is the imbalance of diffusion and sorce terms. The explicit form of Q is not required in the following.

Combined pdf-sdf approach

Finite rate and triple flame regions can now be determined by the level surfaces of the scalar variable $\mathcal{F}$. They are defined implicitly as solutions $\underline{x}$ of

$$S_\mathcal{F}(\varphi, t) \equiv \mathcal{F}(\underline{x}, t) - \varphi = 0 \tag{15}$$

and the unit normal vector of the level surface is defined by

$$n_\alpha \equiv -\frac{1}{|\nabla\mathcal{F}|}\frac{\partial\mathcal{F}}{\partial x_\alpha} \tag{16}$$

pointing into the region where $\mathcal{F} \leq \varphi$ holds, which is regarded as the outward direction since the finite rate regions are on the opposite side of the surfaces. The surface density function is then defined as

$$\Sigma = |\nabla\mathcal{F}|\delta(\mathcal{F}(\underline{x}, t) - \varphi) \tag{17}$$

provided $\mathcal{F}$ is at least once continuously differentiable. The sdf Σ is closely related to the pdf of the scalar $\mathcal{F}$ and its gradient. The scalar pdf f is the expectation of $\delta(\mathcal{F}(\underline{x}, t) - \varphi)$

$$f(\underline{x}, t, \varphi) = \langle\delta(\mathcal{F}(\underline{x}, t) - \varphi)\rangle \tag{18}$$

and it follows then that the expectation of Σ is given by the conditional expectation of the scalar gradient and the scalar pdf

$$\langle\Sigma\rangle(\underline{x}, t, \varphi) = \langle|\nabla\mathcal{F}||\mathcal{F}(\underline{x}, t) = \varphi\rangle f(\underline{x}, t, \varphi) \tag{19}$$

It is straightforward to set up the transport equation (see Pope [4], Candel and Poinsot [2], Trouve and Poinsot [3], Trouve et al. [7]) for the sdf Σ

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial}{\partial x_\alpha}(v_\alpha \Sigma) = (\frac{\partial v_\alpha}{\partial x_\alpha} - n_\alpha n_\beta \frac{\partial v_\alpha}{\partial x_\beta})\Sigma - \delta(\mathcal{F} - \varphi) n_\alpha \frac{\partial \Omega_{\mathcal{F}}}{\partial x_\alpha} - \frac{\partial}{\partial \varphi}(\Sigma \Omega_{\mathcal{F}}) \qquad (20)$$

Averaging produces the equation for the mean sdf

$$\frac{\partial \langle \Sigma \rangle}{\partial t} + \frac{\partial}{\partial x_\alpha}\langle v_\alpha \Sigma \rangle = \langle (\frac{\partial v_\alpha}{\partial x_\alpha} - n_\alpha n_\beta \frac{\partial v_\alpha}{\partial x_\beta})|\nabla \mathcal{F}| - n_\alpha \frac{\partial \Omega_{\mathcal{F}}}{\partial x_\alpha} | \mathcal{F} = \varphi \rangle f(\varphi)$$

$$-\frac{\partial}{\partial \varphi}[\langle \Omega_{\mathcal{F}} |\nabla \mathcal{F}| | \mathcal{F} = \varphi \rangle f(\varphi)] \qquad (21)$$

The mean sdf is generated by the strain rate acting in the tangential plane, the flux of the diffusive-ractive imbalance $\Omega_{\mathcal{F}}$ normal to the surface and the flux of $\Omega_{\mathcal{F}}$ in scalar space. The velocity - scalar pdf $f(\mathrm{v}, \varphi_1, \cdots, \varphi_N, \mathcal{F}, \mathrm{x}, t)$ is governed by (Pope [5],Kollmann [6])

$$\rho \frac{\partial f}{\partial t} + \rho \mathrm{v}_\beta \frac{\partial f}{\partial x_\beta} + \sum_{i=1}^{N} \frac{\partial}{\partial \varphi_i}(\rho Q_i f) = \frac{\partial}{\partial \rho}(\langle \rho^2 \nabla \cdot \mathrm{v} | \mathcal{C} \rangle f)$$

$$+\frac{\partial}{\partial \mathrm{v}_\alpha}(\langle \frac{\partial p}{\partial x_\alpha} - \frac{1}{Re}\frac{\partial \tau_{\alpha\beta}}{\partial x_\beta} | \mathcal{C} \rangle f) - \frac{1}{ReSc}\sum_{i=1}^{N} \frac{\partial}{\partial \varphi_i}\langle \frac{\partial}{\partial x_\beta}(\rho \mathcal{D} \frac{\partial \Phi_i}{\partial x_\beta}) | \mathcal{C} \rangle f) - \frac{\partial}{\partial \varphi}\langle \rho \Omega_{\mathcal{F}} | \mathcal{C} \rangle f) \qquad (22)$$

where the condition is defined by the event $\mathcal{C} \equiv \{v_\alpha = \mathrm{v}_\alpha \wedge \Phi_i = \varphi_i, i = 1, \cdots, N \wedge \mathcal{F} = \varphi\}$ and the N non-conserved scalars Φ describing the local state are governed by pdes in the form of (13). The equations for the pdf and the (mean) sdf pose two major closure problems involving scalar transport: The fluxes in scalar space and the surface mean of the total generation rate of sdf. The flux $\langle \Omega_{\mathcal{F}} |\nabla \mathcal{F}| | \mathcal{F} = \varphi \rangle$ for the scalar pdf is generally split into the mixing model and the chemical reaction term, which can be given a closed expression in many cases. However, mixing and chemical reactions are intimately linked. It can be shown (Vervisch et al. [9]) for the homogeneous case that the transport terms in scalar space are the same physical process averaged in different ways for pdf and sdf equations. Hence a combined pdf-sdf approach holds promise for a unified closure.

Results for 2-d flames

Im and Chen [11] investigated the structure and propagation of triple flames in partially premixed hydrogen-air mixtures using detailed chemistry. These results are used to verify the properties of the scalar variables defined in the previous sections for the detection of finite-rate regions. The case of a strong interaction with a vortex offers a suitable test case. The computational domain was two-dimensional with dimensions of 7.2mm×3.6mm, in which 1001×501 grid resolution is used. A hydrogen-air mixing layer at the ambient condition (300K, 1atm) was initially imposed with a mixing thickness which varied continuously from 2.5% to 50% of the shorter domain length. The initial concentration for the fuel stream was hydrogen diluted with 50% nitrogen by volume. A concentrated Gaussian temperature field

$$T(x,y) = T_0 + (T_{\max} - T_0)\exp[-\{(x-x_c)/\delta\}^2]\exp[-\{(y-y_c)/\delta\}^2] \qquad (23)$$

($T_0 = 300\text{K}$, $T_{\max} = 3000\text{K}$, $\delta = 0.05L_r$) was imposed at the center of the mixing layer to initialize the combustion. The high temperature of the ignition source insures rapid ignition and a pair of triple flames develops propagating along the stoichiometric mixture fraction line in both directions.

The effect of unsteady straining on the structure and propagation of an edge flame was simulated by restarting the solution field at $t/\tau_r = 15$ with a pair of counter-rotating vortices just upstream of each triple flame. The azimuthal velocity profile had the form of a modified Oseen vortex

$$\frac{u_\theta(r)}{u_{\theta,max}} = \frac{\beta\sigma^2}{2\pi r^2}[1 - e^{-(r/\sigma)^3}], \qquad (24)$$

where $r^2 = (x-x_c)^2 + (y-y_c)^2$, σ is the nominal vortex radius, $\beta = 0.9833$. The direction of the vortex pair is such that the triple flame tip is pulled into the channel between the vortices, further details are given by Im and Chen[11] The vortex/edge flame interaction is then used to test the criterion developed for detecting finite-rate regions.

Figure 1 to 3 (time $t = 19$) and fig.4 to 6 ($t = 29$) show the isolines of the scalar $\mathcal{F}$ for three choices of the non-conserved scalar in the vector g: (1) density ρ, (2) mass fraction of H_2O, (3) mass fraction of OH. It is evident that the detailed variation of the scalar $\mathcal{F}$ within the finite rate regions is different for (1) to (3), but the outline (level value f_0 small compared to the maximum) is essentially the same for density and mass fraction of H_2O at both times, but the radical is clearly less suited for the purpose of detection as it is present mostly in lean mixtures. This could be improved according to (5) at the cost of increased complexity of the transport pde for $\mathcal{F}$, but the figures indicate that case (1) using density is a better choice even for complex chemistry.

Conclusions

A new scalar variable based on geometric properties of level surfaces was constructed that allows the detection of finite rate and triple flame regions. It is bounded in the limit of infinitely fast chemistry and can be applied to complex systems of combustion reactions. It is valid for the conditions stated in the assumptions. Evaluation of DNS results showed that various definitions of the scalar using stable mass fractions and density produce the same finite rate region but different distributions of the scalar in them. Radical mass fractions such as Y_{OH} are less suited for the detection since they are not necessarily present in comparable amounts in rich and lean parts of the flow field. A combined pdf-sdf approach was developed that is able to deal with finite rate regions by conditioning with the scalar detecting them.

Acknowledgements

This research was supported by the United States Department of Energy, Office of Basic Energy Sciences, Chemical Sciences Division.

References

[1] Kollmann, W. and Chen J.H., *Twenty-Fifth Symposium (Int.) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1994, pp.1091-1098.

[2] Candel, S.M. and Poinsot, T., *Comb. Sci. Technol.* 70:1-15 (1990).

[3] Trouvé, A. and Poinsot, T., "The evolution equation for the flame surface density density in turbulent premixed combustion", CTR manuscript 140 (1993), Stanford University and NASA Ames.

[4] Pope, S.B., *Int. J. Engng. Sci.* 26:445-469 (1988).

[5] Pope, S.B., *Progr. Energy Combust. Sci.* 11:119-254 (1985).

[6] Kollmann, W., *Theoret. Comput. Fluid Dyn.* 1:249-285 (1990).

[7] Trouve, A., Veynante, D., Bray, K.N.C. and Mantel, T., "The coupling between flame surface dynamics and species mass conservation in premixed combustion", CTR Proc. 1994 Summer Program, pp.95-124.

[8] Vervisch, L., Kollmann, W., Bray, K.N.C. and Mantel, T., "Pdf modeling for premixed turbulent combustion based on the properties of iso-concentration surfaces", CTR Proc. 1994 Summer Program, pp.125-150.

[9] Vervisch, L., Bideaux, E., Bray, K.N.C. and Kollmann, W., *Physics of Fluids* 7:2496-2503 (1995).

[10] Dold, J.W., *Combustion & Flame* 76:71-87 (1989).

[11] Im, H.G. and Chen, J.H., *Combustion & Flame* 119:436-454 (1999).

[12] Linan, A. and Williams, F.A., *Fundamental aspects of combustion*, Oxford University Press, 1993.

[13] Echekki, T. and Chen, J.H., *Combustion & Flame* 114:231-245 (1998).

[14] Hartley, L.J. and Dold, J.W., *Combust. Sci. Technol.* 80:23-46 (1991).

[15] Domingo, P. and Vervisch, L., *Twenty-sixth Symposium (Int.) on Combustion*, The Combustion Institute, Pittsburgh, 1996, pp.233-240.

[16] Majda, A. and Sethian, J., *Combust. Sci. Technol.* 42:185-205 (1985).

[17] Williams, F.A., *Combustion Theory*, Benjamin/Cummings Publ. Comp. Inc., Menlo Park, 1985.

Figure Captions

1. Isolines of $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$ for g constructed with mixture fraction Z and density ρ at time $t = 19$.

2. Isolines of $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$ for g constructed with mixture fraction Z and mass fraction of H_2O at time $t = 19$.

3. Isolines of $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$ for g constructed with mixture fraction Z and mass fraction of OH at time $t = 19$.

4. Isolines of $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$ for g constructed with mixture fraction Z and density ρ at time $t = 29$.

5. Isolines of $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$ for g constructed with mixture fraction Z and mass fraction of H_2O at time $t = 29$.

6. Isolines of $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$ for g constructed with mixture fraction Z and mass fraction of OH at time $t = 29$.

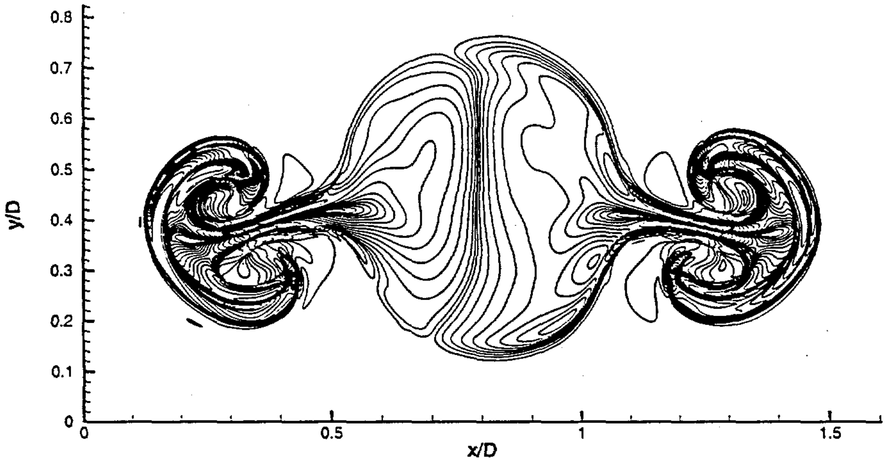

Figure 1: Isolines of $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$ for g constructed with mixture fraction Z and density ρ at time $t = 19$.

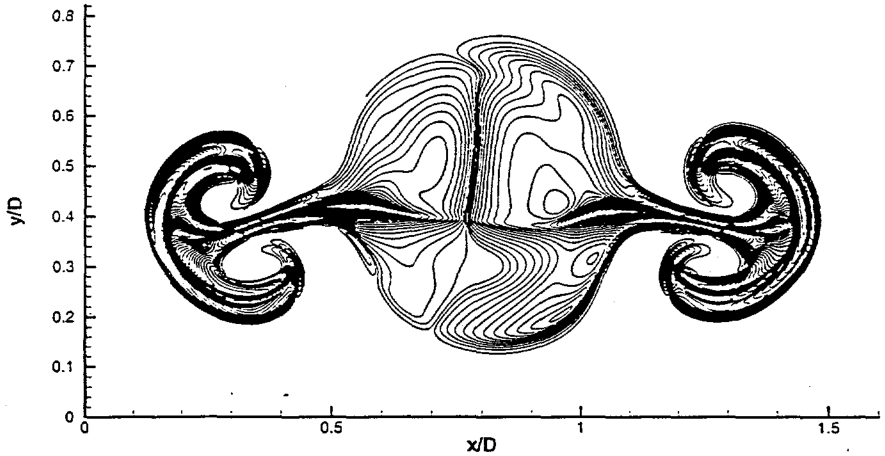

Figure 2: Isolines of $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$ for g constructed with mixture fraction Z and mass fraction of H_2O at time $t = 19$.

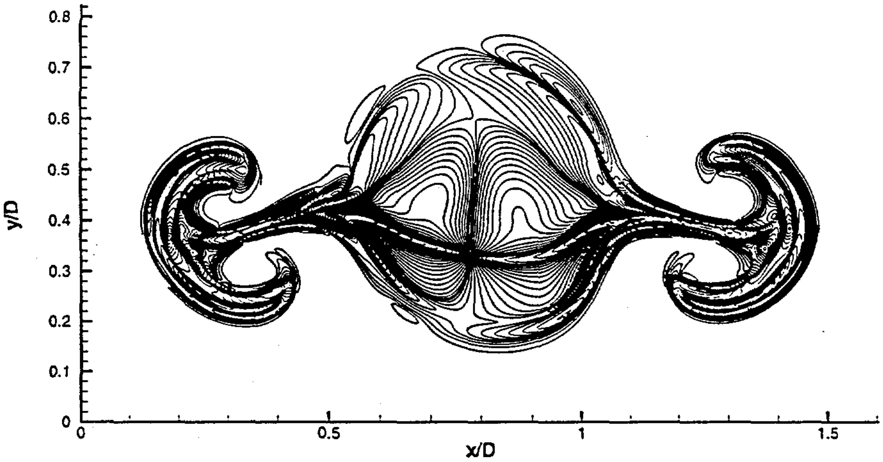

Figure 3: Isolines of $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$ for g constructed with mixture fraction Z and mass fraction of OH at time $t = 19$.

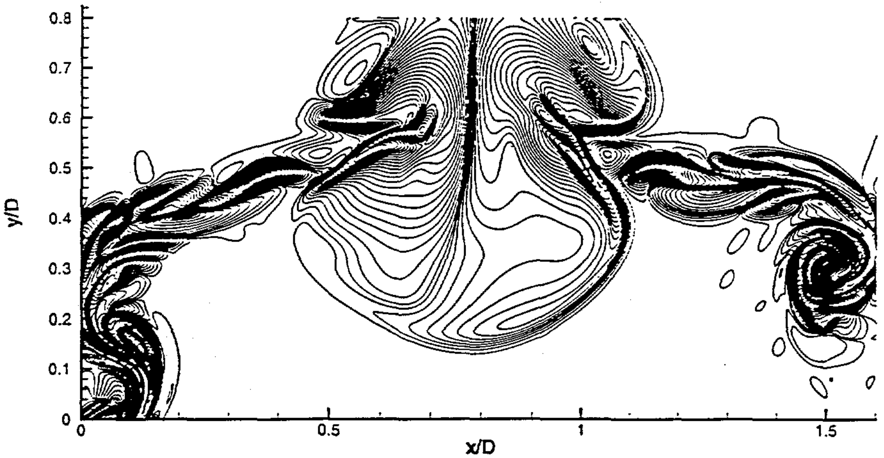

Figure 4: Isolines of $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$ for g constructed with mixture fraction Z and density ρ at time $t = 29$.

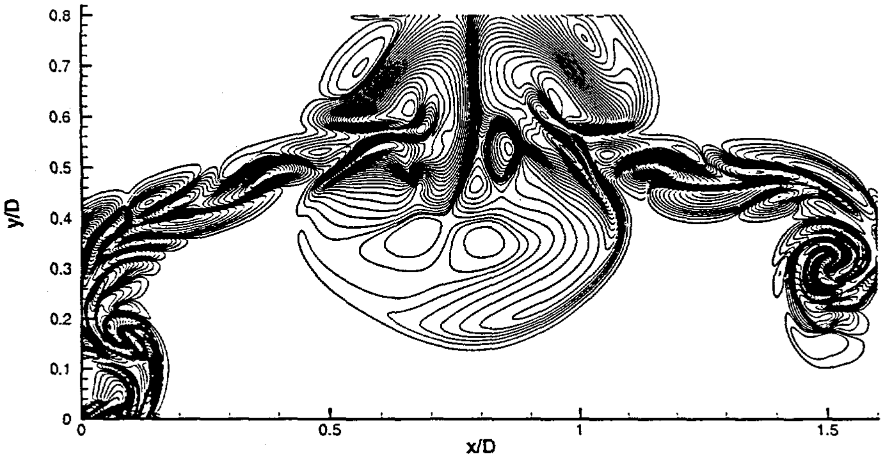

Figure 5: Isolines of $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$ for g constructed with mixture fraction Z and mass fraction of H_2O at time $t = 29$.

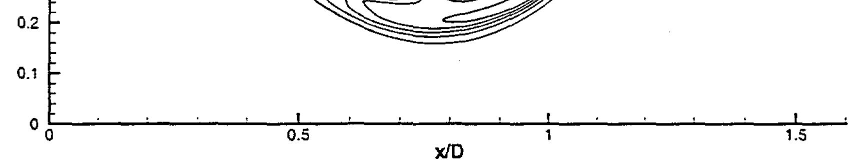

Figure 6: Isolines of $\mathcal{F} = \mathrm{g} \cdot \mathrm{g}$ for g constructed with mixture fraction Z and mass fraction of OH at time $t = 29$.